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UCRL-TR-227019

Nano-focused Bremstrahlung Isochromat Spectroscopy (nBIS) Determination of the Unoccupied Electronic Structure of Pu

J. G. Tobin, M. Butterfield, N. Teslich, A. Bliss, B. Chung, J. Gross, A. McMahan, A. Schwartz

December 29, 2006

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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Nano-focused Bremstrahlung Isochromat Spectroscopy(nBIS) Determination of the Unoccupied Electronic Structure of Pu

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Co-investigators: Martin Butterfield (Post-Doc), Nick Teslich, Ann Bliss, Brandon Chung, James Gross (Summer Student), Andy McMahan (PAT), Adam Schwartz (PAT)

Total Project Original Budget: $500K/year Operations + $500 Capital Equipment

Total Project Budget	CMS-op	DNT-op	Total-op	Cap.Eq
FY04 Budget Requested	$ 0K	$ 0K	$ 0K	$0K
FY04 Budget Received (Starting 7/04)	$ 100K	$ 0K	$ 100K	$300K
FY05 Budget Requested	$ 200K	$ 300K	$ 500K	$500K
FY05 Budget Received	$ 110K	$ 126K	$ 236K	$89K (CMS)
FY06 Budget Requested	$ 200K	$ 300K	$ 500K	$ 0K
FY06 Budget Received	$ 116K	$ 0K	$ 116K	$44K (CMS)
FY07 Budget Requested	$ 200K	$ 300K	$ 500K	$ 0K
FY07 Budget Received	$ 0K	$ 0K	$ 0K	$ 0K
Budget Total Requested	$ 600K	$ 900K	$ 1500K	$500K
Budget Total Received	$ 326K	$ 126K	$ 452K	$433K
Percentage Req/Rec	54%	14%	30%	87%

The proposal was originally put forward in the Spring of 2004, requesting funding in FY05 (Oct 04 – Sep 05), FY 06 (Oct 05 – Sep 06) and FY 07 (Oct 06 – Sep 07). Pre-funding in late FY 04 was provided, beginning in July of 2004.

Outline of Report

I. Description of Original Proposal
II. Description of Progress
III. International Recognition: Publications and Talks
IV. Future Plans
V. Acknowledgements

I. Description of Original Proposal

Introduction:

While chemically toxic and highly radioactive, Pu may be the most scientifically interesting element in the periodic table. It's properties include the following: six different phases, close to each other in energy and sensitive to variations of temperature, pressure and chemistry; the face-centered-cubic phase (delta) is the *least* dense; Pu expands when it solidifies from the melt; and it is clearly the nexus of the actinide binary phase diagrams of the actinides. In a sense, it is the boundary between the light (ostensibly delocalized 5f electrons) and heavy (ostensibly localized or correlated 5f electrons) actinide elements, but this is an over-simplification. The localized atomic 5f states are naturally correlated, but important regimes of correlated electron states are conceivable as extended states on the delocalized side of the possible Mott transition between conductive and insulating behavior. The proximity to this crossover may be the driving force behind all these exotic properties. Pu remains of immense scientific and technological importance and the advancement to a firm, scientific understanding of the electronic structure of Pu and its compounds, mixtures, alloys and solutions is a crucial issue. Moreover, while there are a number of ongoing experimental efforts directed at determining the occupied (valence band, below the Fermi Energy) electronic structure of Pu, there is essential no experimental data on the unoccupied (conduction band, above the Fermi Energy) electronic structure of Pu.

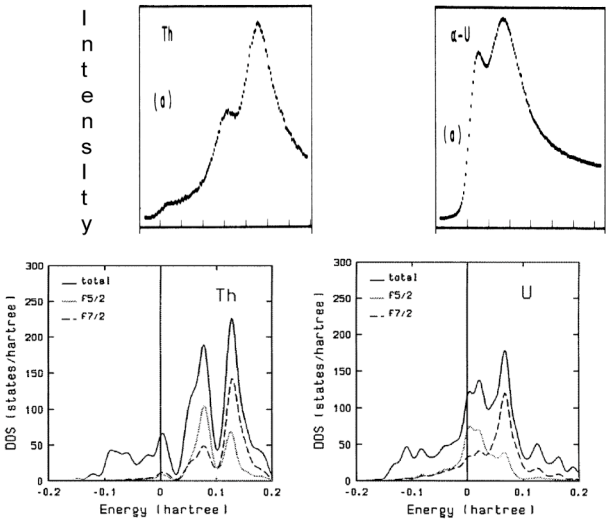
Objective:

Our objective is to determine the conduction band (unoccupied) electronic structure of Pu and other actinides (and possibly rare earths as well), in a phase specific fashion and emphasizing bulk contributions. This is world-class science directed at issue that is central to LLNL and DOE: Pu structure property relationships.

Conduction band (unoccupied) electronic structure is the missing link in studies of Pu. nBIS is the best way to determine the unoccupied electronic structure.

As can be seen in Figure 1 (below), Bremstrahlung Isochromat Spectroscopy (BIS) can provide a direct measure of the unoccupied electronic structure of actinides. Unfortunately, this data only exists for Th and U, not Pu! Moreover, our studies of Pu electronic structure are predicated upon measuring the conduction bands of **bulk** Pu in a **phase specific** fashion. Because of the lack of single crystals of Pu, we will perform our experiments in a nano-focusing fashion, allowing us to interrogate the micro-single-crystalline structures in Pu polycrystalline samples. (We will return to this issue shortly.)

UNCLASSIFIED



← **Unoccupied density of states of Th and U from Bremstrahlung Isochromat Spectroscopy (BIS) by Baer and Lang, PRB 21, 2060 (1980).**

← **Occupied (neg energies) and unoccupied (pos energies) Density of States of Th and U calculated by Penicaud, J. Phys. C. M. 9, 6341 (1990).**

Figure 1: The BIS and calculated electronic structure of Th and U

To get bulk sensitivity, we will follow the lead of Mo et al, who recently demonstrated with photoelectron spectroscopy that higher photon energies are essential to the measurement of bulk properties. (See Figure 2, right.) Finally, we plan to perform these investigations with a nano-focussing spectrometer constructed of off-the-shelf items.

For additional reasons why the study of Pu unoccupied electronic structure is important, please see the attached letter from Andy McMahan and John Moriarity (page 7).

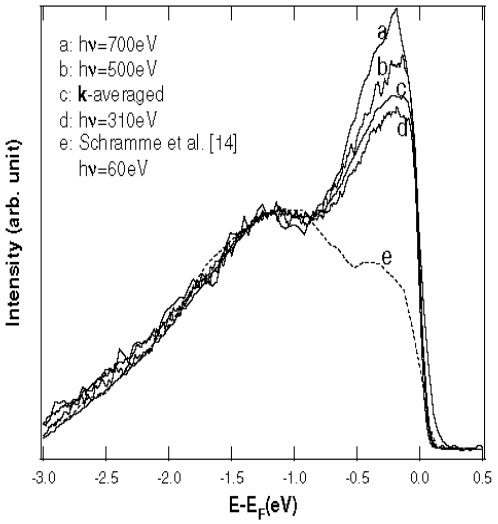


FIG. 2. PES spectra taken with various $h\nu$, the largest of which yields the greatest bulk sensitivity.

Sensitivity to the bulk V_2O_3 quasiparticle peak increases with increasing energy Mo et al, PRL 90, 186403 (2003)]

Experimental Approach

The central technique is BIS or high energy Inverse Photoelectron Spectroscopy.
BIS is the high-energy variant of inverse photoelectron spectroscopy (IPES: electron in, photon out), which is essentially the time reversal of photoelectron spectroscopy (photon in, electron out), as illustrated in Figure 3. IPES can be used to follow the dispersion of electronic states in ordered samples: an example of this is shown in Figure 4. Owing to its low energies (hv ≈ 10 eV), IPES is usually very band and surface sensitive.

However, by working at higher energies, we will sample preferentially for bulk Density of State (DOS) properties, downgrading the impact of surface effects, following a philosophy similar to that of Mo et al, PRL 90, 186403 (2003), as described above. Thus, from BIS, we would have a direct measure of the conduction band or unoccupied electronic structure of the bulk Pu.

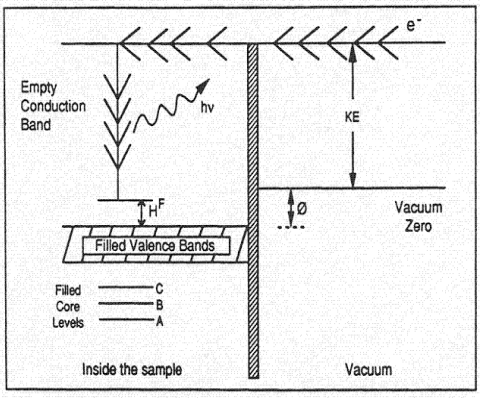


Figure 3 (above): IPES

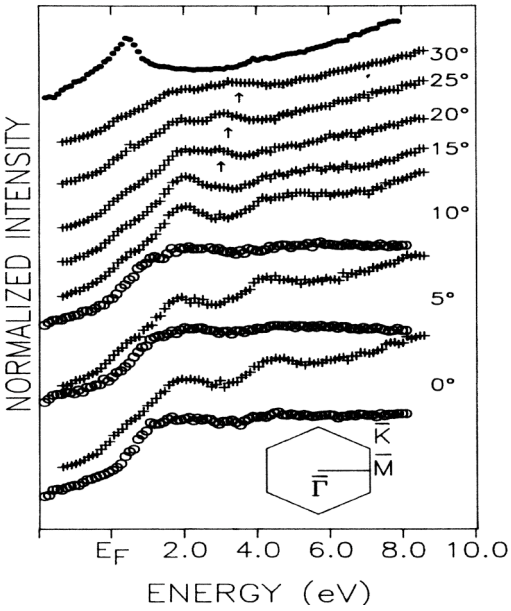


Figure 4 (to the right):
IPES of Ag/Ge(111),
Knapp and Tobin, PRB 37, 8656 (1988).
○ = Ge, + = Ag/Ge, ● = Ag

Using a Scanning Electron Microscope (SEM) as the electron beam source in the BIS process, we would be able to probe the single crystalline micro-crystallites that are available in polycrystalline samples. A major problem with Pu: there are no large single crystals. An alternate approach is to use microscopy to focus in on single crystalline regions within polycrystalline samples, performing spectroscopy on microscopically small single crystals. This approach was used to great success in our previous work with a Transmission Electron Microscope (TEM), as described in "The Failure of Russell-Saunders Coupling in the 5f States of Plutonium", by K.T. Moore, M.A. Wall, A.J. Schwartz, B.W. Chung, D.K. Shuh, R.K. Schulze, and J.G. Tobin, Phys. Rev. Lett. 90, 196404 (May 2003). Please note that there is no ambiguity here about the phase. The electron diffraction provides a direct and irrefutable indication of the crystallinity of the micro-structure.

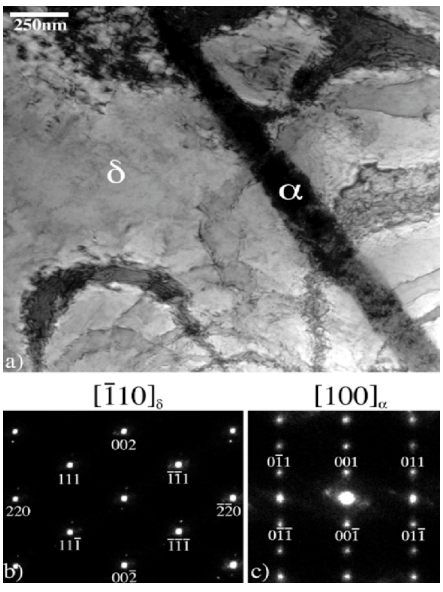


Figure 5 (to the right):
Polycrystalline Pu
Upper: TEM-Microscopy
Lower: Phase Specific Electron Diffraction
Moore et al, PRL 2003.

Technical Description:

We will perform in house experiments with off-the-shelf instrumentation. By setting up as an in house experiment in Bldg 235, we can take advantage of the Pu preparation and handing capabilities therein, i.e. Mark Wall and all of his expertise. We can buy a slightly used SEM to function as the focused electron source. The photon detection will be a commercially available soft x-ray spectrometer, from one of a series of companies that provide monochromators and detectors to synchrotron radiation users.

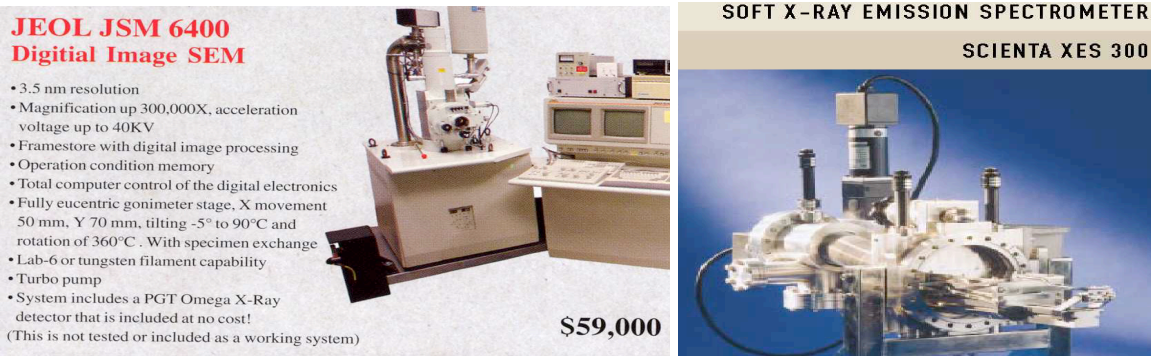


Figure 6:

SEM (above,left panel) and X-ray Emission Spectrometer (XES) (above,right panel)

We will begin our studies using Rare Earths such as Ce and the less radioactive actinides such as depleted Uranium. Ce, the Rare Earth analogue of Pu, has a similar multi-phase electronic structure controversy. The first phase specific spectra of Ce have been recently reported by Moore et al [K.T. Moore, B.W. Chung, S.A. Morton, A.J. Schwartz, J.G. Tobin, S. Lazar, F.D. Tichelaar, H.W. Zandbergen, P. Söderlind, and G. van der Laan, "Changes in the electronic structure of cerium due to variations in close packing," Phys. Rev. B **69**, 193104 (2004)]: will we build upon that and use the Ce study to prepare us for the more difficult case of Pu.

Science Impact:

We will resolve 4f and 5f Electronic Structure issue by comparing directly our results to the predictions of Dynamical Mean Field Theory (DMFT) such as that of Pu by Savrosov et al [Nature 410, 793 (2001)] and Ce by Held, McMahan and Scarlettar [PRL 87, 276404 (2001)]

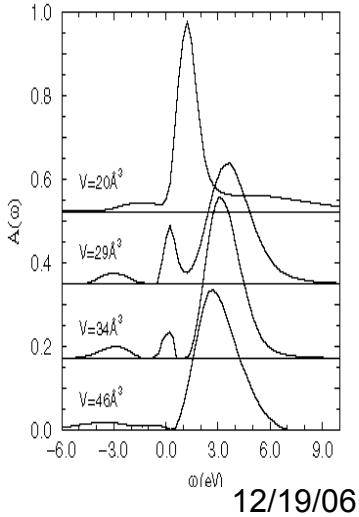


Figure 7 (to the right):
Ce data from Held, McMahan and Scarlettar: Test for the f^1 ($\omega \cong 0$ eV) and f^2 ($\omega \cong 3$ eV) final state features in the nBIS spectra.

Technology Impact & Exit

We will provide the following:

(1)Validation of Pu Equation of State (EOS) Theories;

(2)Benchmarking of modeling for science-based stockpile stewardship;

(3) a strengthening of Pu Science within the Strategic Planning Theme Area (MPPXC:Actinides);

(4) a contribution to the scientific infrastructure for programmatic work (after the LDRD ends, this instrumentation becomes part of part of the CMS Center for Actinide Material Science and Technology).

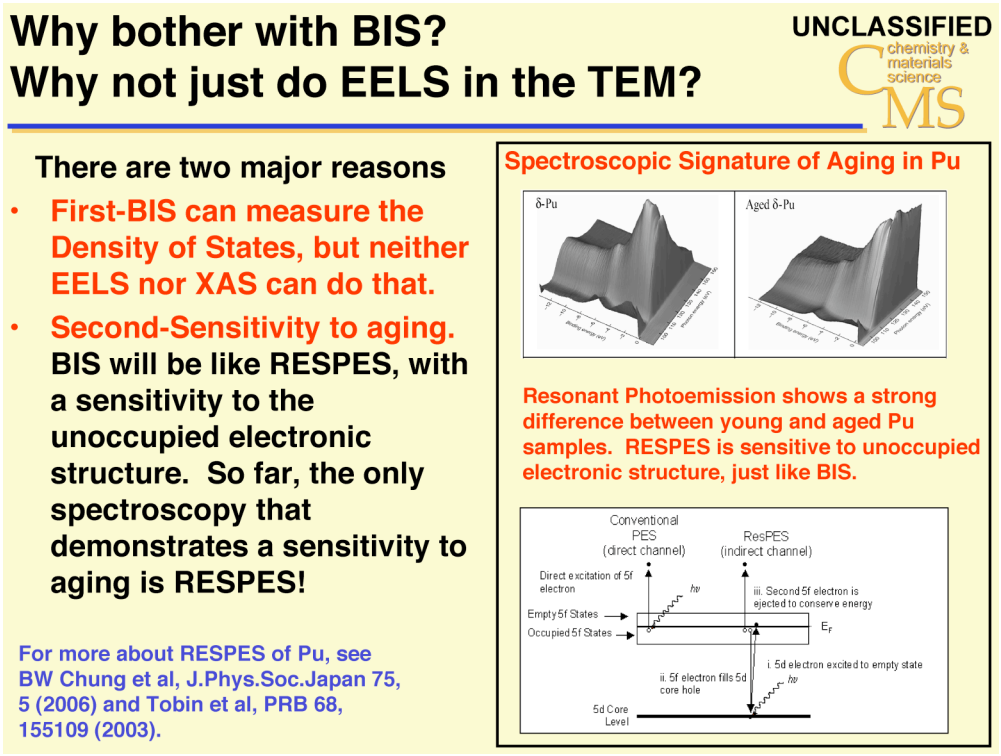


Figure 8

Proposal Summary

We will determine the conduction band (unoccupied) electronic structure of Pu and other actinides (and possibly rare earths as well), in a phase specific fashion and emphasizing bulk contributions. This is world-class science directed at issue that is central to LLNL and DOE: Pu structure property relationships

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Addendum: Support outside of CMLS for the BIS approach.

Interdepartmental Letterhead

Mail Station: L-045

Ext: 2-7198

H DIVISION

Aug 6, 2003

TO: Jim Tobin

FROM: Andy McMahan, John Moriarty

SUBJECT: **Brehmstrahlung Isochromatic Spectrometer**

Equation of state in the implosion regime depends predominantly on the underlying electronic structure. While spectroscopic techniques do not directly give equation of state, they probe the electronic structure and can therefore constrain theoretical treatments which do yield equation of state, and provide a clearer understanding of the fundamental physics involved. In particular spectroscopic techniques can help sort out and constrain a variety of important factors including normal itinerant banding effects, Hubbard and spin-orbit splitting, and atomic-like term structure in the more localized regimes.

There has been much recent Photoemission Spectroscopy (PES) activity for plutonium which probes the occupied states, and issues of surface effects including both impurities and reconstruction are in the process of being resolved. Unfortunately there has been almost no work in recent years probing the unoccupied states with "inverse photoemission" or Brehmstrahlung Isochromatic Spectroscopy (BIS). This is unfortunate since the addition of the empty state spectra more than doubles the impact of the combined data, since its knowledge also constrains interpretation of the PES and vice versa. There is no doubt that precise and reliable combined PES/BIS data for the various phases of Pu will have both important scientific and programmatic impact. Among issues that such data will help resolve is the degree of localization or itineracy in the 5f electrons in a variety of Pu phases: pure α-Pu, the Ga-stabilized δ phase, the pure high-temperature δ phase, and the other high-temperature phases (β, γ, δ', and ε).

In summary, we believe the development of a BIS capability at the Laboratory is important, and should be supported.

II. Description Of Progress:

ACCOMPLISHMENT 1: Lab setup and SEM operational

An SEM was purchased and set up in Room 1210, B235. Room 1210 was modified to be compatible with the incoming nBIS experiment. Below, one can see a micrograph taken with the SEM of gold particles on graphite, in Room 1210, B235.

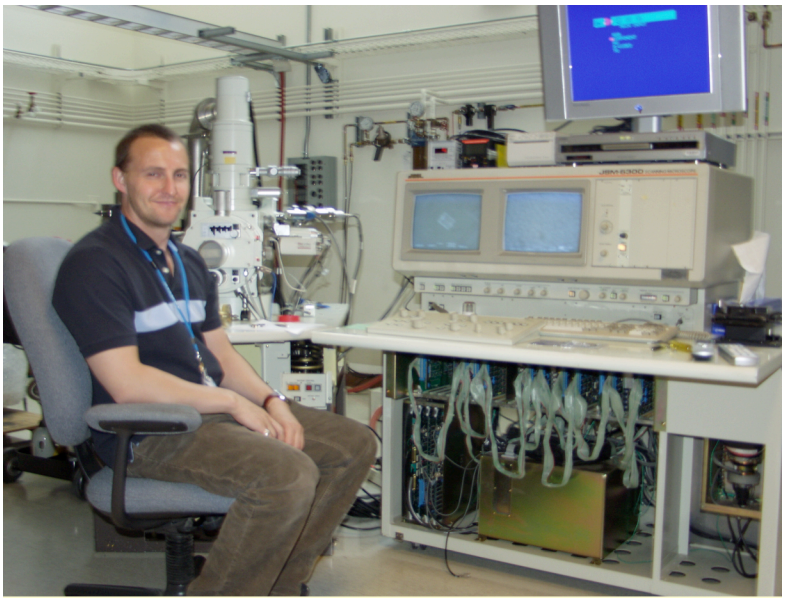


Figure 9

Martin Butterfield is shown seated at the operational SEM in Room 1210, B235

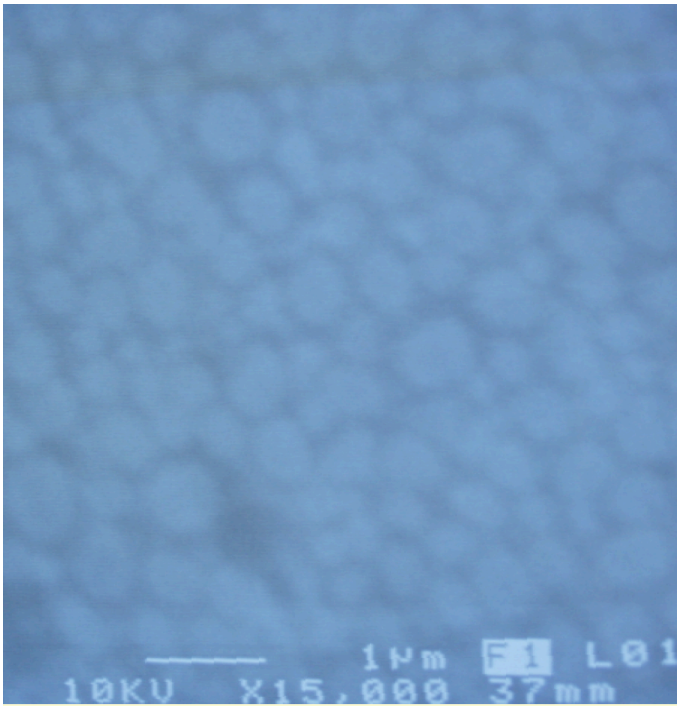


Figure 10

Micrograph of Au particles on graphite, taken on the operation SEM in Room 1210, B235.

ACCOMPLISHMENT 2: Integration of SEM and XES350

We had made substantial progress in designing our new UHV system for housing the nBIS experiment, combining both the spatial resolution of the SEM with the ultra high vacuum necessary for Pu experiments. An array of vacuum pumps and hardware had already been purchased.

This design work was done by Martin Butterfield (Post-doc) and James Gross (Summer Student), under the guidance of JGT.

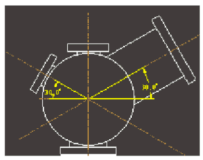
Figure 11 (right)

Design of the new vacuum vessel for UHV work, optimized to match with the extant SEM and XES-350 instrumentation.

Top View of nBIS chamber

Flange 2
•4.5 inch OD ConFlat
•6 inches from flange face to centerline
•on y axis
•window mounted here

Flange 3
•4.5 inch OD ConFlat
•6 inches from flange face to centerline
•30 degrees off of x axis
•EDAX EBSD Detector and retractor mounted here
•miminum distance from flange face of EDAX to centerline is 8.2 inches



Flange 1
•8 inch OD ConFlat
•11.2 inches from flange face to centerline
•30 degrees off of x axis
•XES 350 mounted here

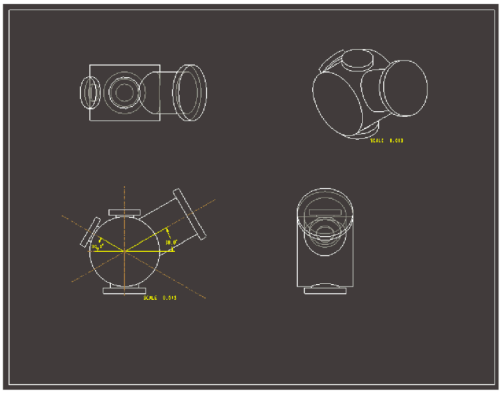
Flange 4
•6 inch OD ConFlat
•6 inches from flange face to centerline
•on y axis
•sample manipulator mounted here

Side View of nBIS chamber

Flange 5
•10 inch OD ConFlat
•4 inches from flange face to center-plane
•z axis
•SEM source mounted here

Flange 6
•10 inch OD ConFlat
•4 inches from flange face to center-plane
•z axis
•Pumping manifold mounted here

Overall design



ACCOMPLISHMENT 3: XES350 On site and Operational

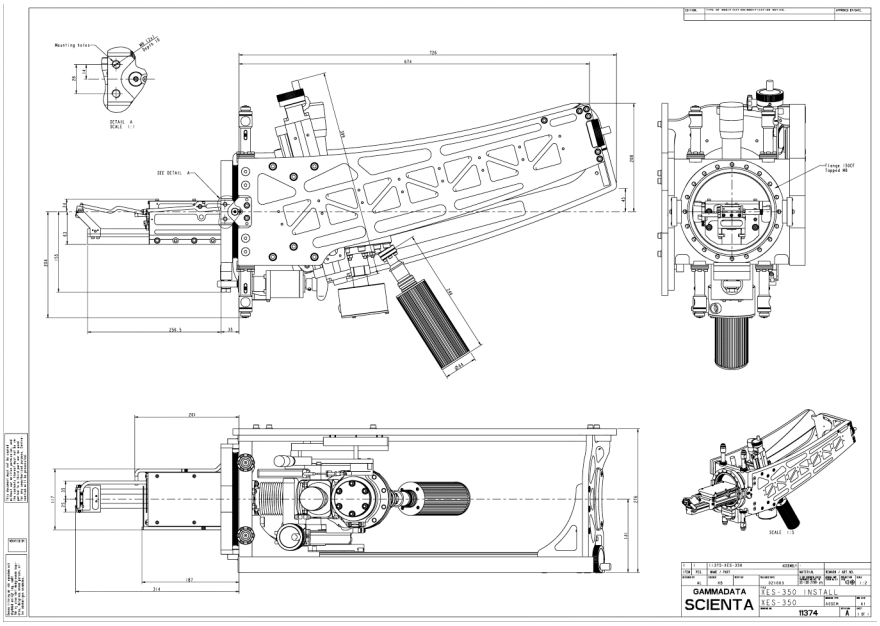


Figure 12
XES350 monochromatic photon detection system from Gamma Data Scienta

The Monochromatic Photon Detection Is Functional.

The photon detection was to be performed with a commercially available soft x-ray spectrometer, the XES350 that we had already purchased from Gammadata Scienta. The 3 gratings for the XES350 give us an energy window of 50-1500 eV, thereby allowing us to concentrate on bulk properties, but also compare and contrast with any surface related features. Results of our preliminary testing of the XES-350 are shown below. These spectra were collected on site in B235.

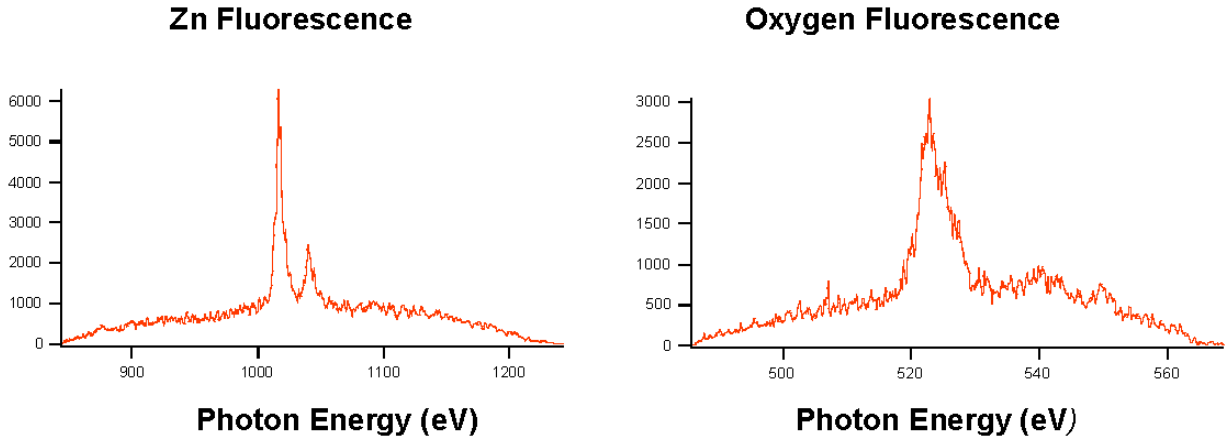


Figure 13
Electron stimulated fluorescence, using an electron excitation beam energy of 3000 eV.

(Left) Zn 2p doublet . (Right) O1s. Data collected on site in B235.

ACCOMPLISHMENT 4: Safety Plan Development and Approval

IWS Summary:

HELP

IWS #:	WAL:	Int Start Date:	Est Comp Date:
12605 r8	B	01-APR-05	On-Going

Title:

Installing and testing of SEM and X-ray spectrometer

Description:

Installation, troubleshooting and testing of a scanning electron microscope (SEM) and X-ray Spectrometer for nanoscale Brehmstrahlung Isochromat Spectroscopy experiments. No hazardous or radioactive waste will be generated under this IWS. Used wipers are evaluated at end of process, are dry, and are disposed in the municipal trash.

Authorizing Organization:	Authorizing Individual:
AD - Chemistry and Materials Science	GDOWSKI, TAMMY S
Responsible Individual:	**Submitter:**
BUTTERFIELD, MARTIN T	LOGRANDE, ROBERTA M

Concurrence Statuses:

Loc • Fac/Wing • Room • Team	ES&H	FAC	Add Con Loc	RI	Add Con IWS	AI
LLNL-Facility • 235 • 1210 • ES&H Team 5	CONCUR 14-APR-05 Simpson	CONCUR 28-APR-05 Beckett	N/A	CONCUR 14-APR-05 Butterfield	CONCUR 28-APR-05 Wall	AUTHORIZED 13-MAY-05 Gdowski

Figure 14 Approved IWS

IWS Summary:

HELP

IWS #:	WAL:	Int Start Date:	Est Comp Date:
13042 r1	B	21-OCT-05	On-Going

Title:

Testing of Photoemission chamber for Brehmstralung Isochromat Spectroscopy (BIS) Experiments

Description:

Assemble and check-out vacuum system and supporting mechanical systems; Testing of components for BIS experiments will be carried out in a vacuum chamber in B235 R1210 using an electron gun. This will involve testing an analyzer purchased from Gammedata Scienta, using an electron gun as an excitation source, and also Photoelectron Spectroscopy, sample preparation by sputtering, instrument development and other related activities. Sample materials used will be transition metals (copper and nickel) and rare earth (Cerium).

Authorizing Organization:	Authorizing Individual:
AD - Chemistry and Materials Science	BLOBAUM, KERRI JAYNE M
Responsible Individual:	**Submitter:**
BUTTERFIELD, MARTIN T	BUTTERFIELD, MARTIN T

Concurrence Statuses:

Loc • Fac/Wing • Room • Team	ES&H	FAC	Add Con Loc	RI	Add Con IWS	AI
LLNL-Facility • 235 • 1210 • ES&H Team 5	CONCUR 09-DEC-05 Simpson	CONCUR 12-JAN-06 Cooper	N/A	CONCUR 02-NOV-05 Butterfield	N/A	AUTHORIZED 17-JAN-06 Blobaum

Figure 15 Approved IWS

IWS Summary:

HELP

IWS #:	WAL:	Int Start Date:	Est Comp Date:
13042.01	B	21-OCT-05	On-Going

Title:

Testing of Photoemission chamber for Brehmstralung Isochromat Spectroscopy (BIS) Experiments

Description:

Assemble and check-out vacuum system and supporting mechanical systems; Testing of components for BIS experiments will be carried out in a vacuum chamber in B235 R1210 using an electron gun. This will involve testing an analyzer purchased from Gammedata Scienta, using an electron gun as an excitation source, and also Photoelectron Spectroscopy, sample preparation by sputtering, instrument development and other related activities. Sample materials used will be transition metals (copper and nickel) and rare earth (Cerium).

Authorizing Organization:	Authorizing Individual:
AD - Chemistry and Materials Science	BLOBAUM, KERRI JAYNE M
Responsible Individual:	**Submitter:**
BUTTERFIELD, MARTIN T	BUTTERFIELD, MARTIN T

Concurrence Statuses:

Loc • Fac/Wing • Room • Team	ES&H	FAC	Add Con Loc	RI	Add Con IWS	AI
LLNL-Facility • 235 • 1210 • ES&H Team 5	CONCUR 26-JAN-06 Simpson	CONCUR 03-FEB-06 Cooper	N/A	CONCUR 30-JAN-06 Butterfield	N/A	AUTHORIZED 03-FEB-06 Blobaum

Figure 16 Approved IWS

IWS Summary:

HELP

IWS #:	WAL:	Int Start Date:	Est Comp Date:
13652 r7	B	21-OCT-05	On-Going

Title:

Testing of Photoemission chamber for Brehmstralung Isochromat Spectroscopy (BIS) Experiments

Description:

Assemble and check-out vacuum system and supporting mechanical systems; Testing of components for BIS experiments will be carried out in a vacuum chamber in B235 R1226 using an electron gun. This will involve testing an analyzer purchased from Gammedata Scienta, using an electron gun as an excitation source to carry out Bremstrahlung Isochromat Spectroscopy experiments, and also Photoelectron Spectroscopy, sample preparation by sputtering, instrument development and other related activities. Sample materials used will be transition metals (copper and nickel) and rare earth (Cerium).

Authorizing Organization:	Authorizing Individual:
Chemistry, Materials, & Life Sciences Directorate	BLOBAUM, KERRI JAYNE M
Responsible Individual:	**Submitter:**
BUTTERFIELD, MARTIN T	GDOWSKI, TAMMY S

Concurrence Statuses:

Loc • Fac/Wing • Room • Team	ES&H	FAC	Add Con Loc	RI	Add Con IWS	AI
LLNL-Facility • 235 • 1210 • ES&H Team 2	CONCUR 08-SEP-06 Simpson	CONCUR 08-SEP-06 Cooper	N/A	CONCUR 08-SEP-06 Butterfield	N/A	AUTHORIZED 11-SEP-06 Blobaum
LLNL-Facility • 235 • 1226 • ES&H Team 2	CONCUR 08-SEP-06 Simpson	CONCUR 08-SEP-06 Cooper	N/A			

Figure 17 Approved IWS

IWS Summary:

HELP

IWS/SP #:	WAL:	Int Start Date:	Est Comp Date:
12757	C	01-MAR-06	On-Going

Title:

nBIS of Pu and the Actinides

Description:

nano Bremstrahlung Isochromat Spectroscopy (nBIS) Investigations of materials such as Pu, U, Th and their alloys, compounds and solutions will be carried out in Room 1210 in B235, under LLNL, DOE and UC Guidelines. This includes spectroscopy data collection such as inverse and direct photoelectron spectroscopy, x-ray absorption spectroscopy etc, sample preparation, instrument development and other related activities. For non-radioactive samples, we have in place IWS 11035. Sample handling and preparation at LLNL will be carried out by Mark Wall under IWS 10439 using the type III radiological workplace in Building 235. The samples prepared in this workplace will be transported directly to Room 1210, and when samples are returned to Mark Wall, they may only be unpackaged in a type III radiological workplace. No hazardous or radioactive waste is expected to be generated.

Authorizing Organization:	Authorizing Individual:
Chemistry, Materials, & Life Sciences Directorate	BLOBAUM, KERRI JAYNE M
Responsible Individual:	**Submitter:**
TOBIN, JAMES G	TOBIN, JAMES G

Concurrence Statuses:

Loc • Fac/Wing • Room • Team	ES&H	FAC	Add Con Loc	RI	Add Con IWS	AI
Other DOE Site • 235 • 1210 • ES&H Team 5	DRAFT 13-JUN-05 Simpson	N/A	N/A	DRAFT 13-JUN-05 Tobin	N/A	DRAFT 13-JUN-05 Blobaum

Figure 18 Draft IWS for Radioactive Samples

IV. International recognition: Publications and talks

Publications in print: Conference Proceedings

- J.G. Tobin, M.T. Butterfield, N.E. Teslich Jr., R.A. Bliss, M.A. Wall, A.K. McMahan, B.W. Chung and A.J. Schwartz, "Using Nano-focussed Bremstrahlung Isochromat Spectroscopy (nBIS) to Determine the Unoccupied Electronic Structure of Pu," in "Recent Advances in Actinide Science," Royal Society of Chemistry, ed. R. Alvarez, N.D. Bryan and I. May, page 773 (2006).
- J.G. Tobin, K.T. Moore, B.W. Chung, M.A. Wall, A.J. Schwartz, B.B. Ebbinghaus, M.T. Butterfield, N.E. Teslich Jr. , R.A. Bliss, S.A. Morton, S.W. Yu, T. Komesu, G.D. Waddill, G. van der Laan, and A.L. Kutepov, "Experimental Benchmarking of Pu Electronic Structure," Matl. Res. Soc. Symp. Proc. **893**, 79 (2006).
- M.T. Butterfield, J.G. Tobin, N.E. Teslich Jr, R.A. Bliss, M.A. Wall, A.K. McMahan, B.W. Chung, A.J. Schwartz, and A.L. Kutepov, "Utilizing Nano-focussed Bremstrahlung Isochromat Spectroscopy (nBIS) to Determine the Unoccupied Electronic Structure of Pu," Matl. Res. Soc. Symp. Proc. **893**, 95 (2006).

Presentations

International Invited talks

- JG Tobin, "Using Nano-focused Bremstrahlung Isochromat Spectroscopy (nBIS) to Determine the Unoccupied Electronic Structure of Pu," CEA-NNSA Workshop, Paris, France, June 2005, invited talk.

- J.G. Tobin, "Utilizing Nano-focused Bremstrahlung Isochromat Spectroscopy (nBIS) to Determine the Unoccupied Electronic Structure of Pu ," 5th International Workshop: "Fundamental Plutonium Properties" VNIITF, Snezhinsk, Chelyabinsk Region, Russia, September 12 -16, 2005, invited talk.

International Contributed Presentations

- JG Tobin et al, "Using Nano-focused Bremstrahlung Isochromat Spectroscopy (nBIS) to Determine the Unoccupied Electronic Structure of Pu," Journees des Actnides Conference, Baden/Wien, Austria, April 2005, contributed talk.

- JG Tobin et al, "Nano-focused Bremstrahlung Isochromat Spectroscopy (nBIS) Determination of the Unoccupied Electronic Structure of Pu," Actinides 2005 Meeting, Manchester, UK, July 2005, contributed poster.

- M.T. Butterfield, J.G. Tobin, N.E. Teslich Jr, R.A. Bliss, M.A. Wall, A.K. McMahan, B.W. Chung, A.J. Schwartz and A.L.Kutepov, "Nano-focussed Bremstrahlung Isochromat Spectroscopy (nBIS) to Determine the Unoccupied Electronic Structure of Pu" Journees des Actnides Conference, Oxford, UK, April 2006 contributed poster.

Contributed Presentations

- MT Butterfield, JG Tobin, NE Teslich Jr, RA Bliss, MA Wall, A. McMahan, BW Chung, AJ Schwartz and A LKutepov, "Utilizing Nano-focussed Bremstrahlung Isochromat Spectroscopy (nBIS) to Determine the Unoccupied Electronic Structure of Pu" MRS Fall Meeting 2005, Actinides II Symposium, contributed talk.

IV. Future Plans

It is important that we find some way to continue the nBIS or BIS experiment.

BIS and the unoccupied states may be the key to differentiating between the many different theories of Pu electronic structure. (Figure 19)

BIS may provide the last piece of the puzzle in our ongoing effort to resolve the Pu electronic structure controversy. We have had some success in the past, as illustrated in Figure 20.

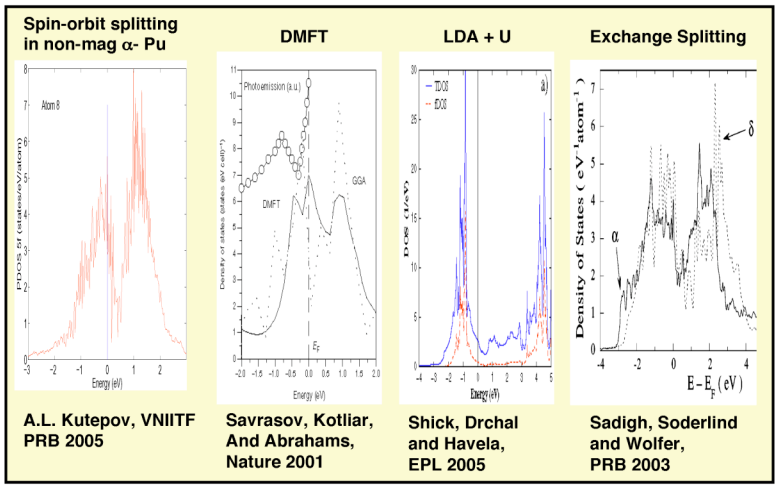


Figure 19
A comparison of the predictions of the unoccupied electronic structure of Pu, from a number of different theoretical approaches is shown here. Many of the theoretical predictions are significantly different.

V.

Acknowledgements

This work was performed under the auspices of the U. S. Department of Energy (DOE) by the University of California, Lawrence Livermore National Laboratory (LLNL) under Contract No. W-7405-Eng-48. The project, 04-ERD-105, was funded by the Laboratory Directed Research and Development Program at LLNL.

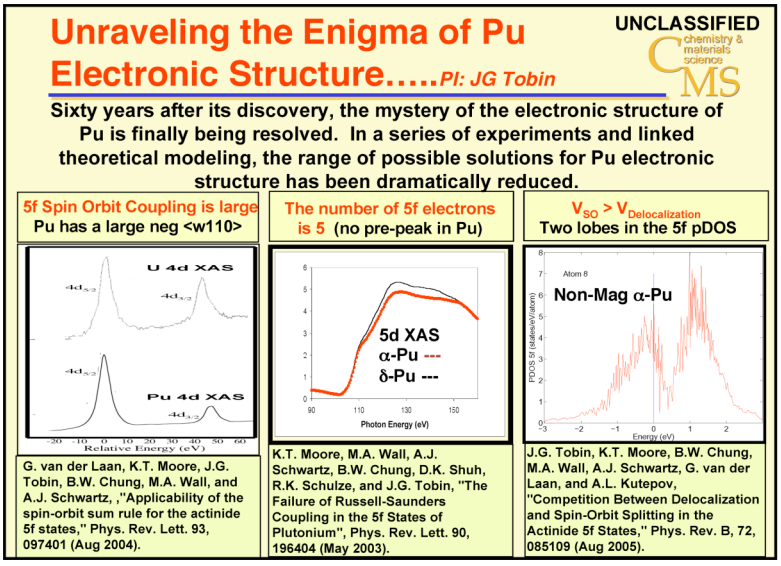


Figure 20